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Bruce Brandt, Director, DC Field Facilities

The instrumentation available to users is always being improved, sometimes in small ways, sometimes by the addition of completely new capabilities. The demand for the Sub-Millimeter Wave Spectroscopy facility for experiments in biology, chemistry, and physics has increased steadily since it was first described in this newsletter about two years ago (*NHMFL Reports, Summer 2002*). Papers describing the results have appeared in *JACS, Phys. Rev., Phys Rev. Letters*, and other journals. Sergei Zvyagin wrote the article below about one of those projects, which exploits some very old ideas to understand a very new problem. The results, just published in the *Physical Review Letters*, suggest that copper pyrimidine dinitrate, a new molecular magnet, is the best candidate to date for studying solitary wave dynamics on the quantum level.

Solitary Waves in Quantum Spin Chains

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The term "soliton" was introduced in the 1960's; however, the scientific research of solitons started in the 19th century when a Scottish engineer and scientist John Scott Russell (1808-1882) observed a large solitary wave while watching wave propagation in shallow water on Union Canal at Hermiston near Edinburgh. Following this discovery, Russell built a 30 ft. wave tank in his backyard and made further important observations on properties of solitary waves that he called Waves of Translation. In the days of Russell, there was much debate concerning the very existence of this kind of solitary wave.

Nowadays, many differential nonlinear equations are known to possess soliton solutions. The sine-Gordon equation

$$\left(\frac{\partial^2}{\partial t^2}\phi(x,t)\right)-\left(\frac{\partial^2}{\partial x^2}\phi(x,t)\right)+\sin(\phi(x,t))=0$$

is one of the most famous "soliton" equations, which is used for a description of a broad class of nonlinear phenomena (see for instance, Ref. 1 and references therein): self-focusing refraction in atom and molecular lasers, magnetic-flux dynamics in Josephson junctions, light propagation in ultrafast fiber-optical intercontinental communication systems, formation of black holes, and even energy transport in biomolecules. The availability of the exact solutions for the sine-Gordon model (soliton, antisoliton, and multiple soliton-antisoliton bound states called breathers) allows a very precise theoretical description of many observable properties and physical parameters of sine-Gordon systems.

On the quantum level the sine-Gordon model is one of the paradigms of the quantum field theory. One of the most basic quantum-mechanical systems is a uniform chain of antiferromagnetically (AFM) coupled S=1/2 spins. Since the S=1/2 AFM chain is critical, even small perturbations can considerably change fundamental properties of the system. One of the most prominent examples is an S=1/2 AFM chain perturbed by an alternating g-tensor and/or the Dzyaloshinskii-Moriya interaction; this situation is realized experimentally in several spin chain systems.[2] In the presence of such

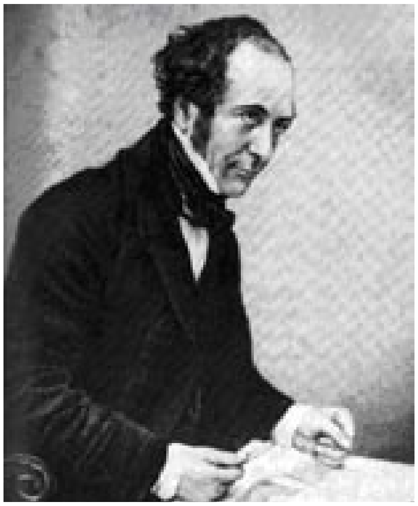

Figure 1. John Scott Russell, a Scottish engineer and scientist, who discovered solitary waves.

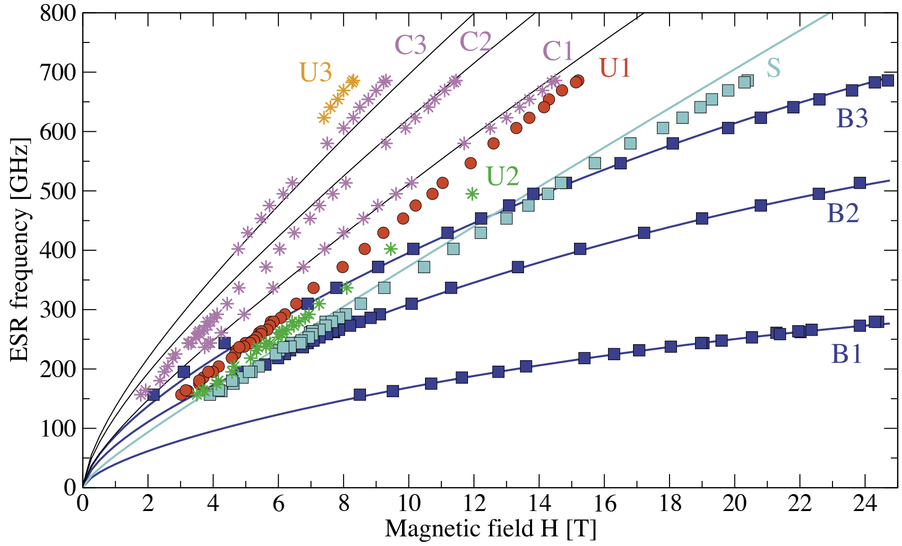

Figure 2. The frequency-field diagram of the ESR modes in Cu-PM. Symbols denote experimental results and lines corresponds to contributions from specific excitations as predicted by the sine-Gordon quantum field theory: the mode S corresponds to soliton excitations, the modes B1-B3 correspond to breather excitations.

interactions, application of a uniform external field H induces an effective transverse staggered field $h \sim H$, which leads to the opening of an energy gap $\Delta \sim H^{2/3}$. The gapped phase can be effectively described by the quantum sine-Gordon field theory recently developed by Oshikawa and Affleck.[3] They predicted a rich solitary wave excitation spectrum consisting of solitons and breathers.

Our study was a detailed investigation of the elementary excitation spectrum in the molecular magnet copper pyrimidine dinitrate (Cu-PM). It has been recently identified as an S=1/2 antiferromagnetic chain system with a field-induced spin gap, and appears to be the best realization of the quantum sine-Gordon spin chain model known to date. The excitation spectrum was studied using a high-field tunable-frequency submillimeter wave electron spin resonance (ESR) spectrometer, recently developed at the National High Magnetic Field Laboratory, Tallahassee.[4]

The complete frequency-field diagram of magnetic excitations in Cu-PM is presented in Fig. 2. *Ten* ESR modes were resolved in the low-temperature spectrum, and their excitation diagram was systematically studied in a broad frequency-field range. For the first time, the field-induced gap in Cu-PM has been observed *directly*. We showed that the size of the gap was determined by excitation energy of the first breather (mode B1, Fig. 2). By comparing the entire set of data with theoretical predictions,[3] we have provided clear experimental evidence for a number of excitations: one soliton (S), three breathers (B1-B3), and several soliton-breather bound excitations (C1-C3) have been observed. The origin of the modes U1-U3 still remains unexplained. Thus, for the first time a complete set of excitations predicted by the sine-Gordon quantum field theory in a quantum spin chain has been confirmed experimentally. It is amazing that waves in shallow water and in quantum spin chains have so much common in their behavior . . .

For more information see S.A. Zvyagin, *et al.*, *Phys. Rev. Lett.*, **93**, 027201 (2004).

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[1] D.K. Cambell, *et al., Physics Today*, **57**, 43 (2004).

[2] D.C. Dender, *et al.*, *Phys. Rev. Lett.*, **79**, 1750 (1997); R. Feyerherm, *et al.*, *J. Phys.: Condens. Matter*, **12**, 8495 (2000); M. Kenzelmann, *et al.*, *Phys. Rev. Lett.*, **93**, 017204 (2004).

[3] M. Oshikawa and I. Affleck, *Phys. Rev. Lett.*, **79**, 2883 (1997); I. Affleck and M. Oshikawa, *Phys. Rev. B*, **60**, 1038 (1999), *ibid.* **62**, 9200 (2000).

[4] S.A. Zvyagin, *et al.*, *Phys. B: Condens. Matter*, **346**, 1 (2004).